

**NCI compounds (Standard agents and compounds with an with sufficient quantities for *in vivo* testing.**

The list contains 365 compounds.

Some compounds may have restriction on distribution (may be due to IP issues or limited inventory)

Many of the compounds have been tested at NCI. The color coding indicates the type of test performed at NCI.

60 cell

hollow fiber

xenografts

**Disclaimer:** The mechanism of action for the majority of these compounds has not been verified by NCI. For many compounds a PubMed ID is given for a reference that supports the indicated mechanism. Some compounds may have activities in addition to those listed here.

| Snd Agent | NSC    | Name   | Activity  | Abbrev       | Source                        | Potentially Restricted Distribution |
|-----------|--------|--|---|--------------|-------------------------------|-------------------------------------|
|           | 93819  | Valproic acid  | Modulates organisation and dynamics of the actin cytoskeleton   | Actin        | PMID: 10098937                |                                     |
|           | 613009 | Jasplakinolide   | Induces overpolymerization of actin.  | Actin        | PMID: 9788576                 | Yes                                 |
| Yes       | 218321 | 2'-deoxycoformycin ;pentostatin  | Blocks adenine deaminase  | ADA          | PMID: 10611432                |                                     |
|           | 6170   | Citral   | Inhibitor of retinoic acid biosynthesis and aldehyde dehydrogenase  | ALDH ; Redox | PMID: 10411631                |                                     |
| Yes       | 79037  | CCNU   | Alkylating Agent  | Alkyl        | PMID: 2818619                 |                                     |
| Yes       | 409962 | BCNU   | Alkylating Agent  | Alkyl        |                               |                                     |
| Yes       | 118742 | Pentamethylmelamine  | Alkylating agent  | Alkyl        | PMID: 3882257                 |                                     |
| Yes       | 95466  | PCNU   | Alkylating Agent  | Alkyl        | PMID: 1998983                 |                                     |
| Yes       | 85998  | Streptozoticin   | Alkylating agent; MGMT knockout mouse has increased sensitivity   | Alkyl        | PMID: 10375003                |                                     |
| Yes       | 45388  | Dacarbazine  | DNA-methylating drug  | Alkyl        | PMID: 9816173                 |                                     |
| Yes       | 283162 | Trimethyl TMM  | analog of nsc13875: Appears to require metabolic activation. Metabolic intermediates may act as alkylating agents | Alkyl        |                               |                                     |
| Yes       | 278214 | Carbamic acid, 1-methylethyl-, [5-(3,4-dichlorophenyl)-2, 3-dihydro-1H-pyrrolizine-6,7-diyl]bis(methylene) ester | analog of nsc89241: DNA-Directed alkylating agent   | Alkyl        |                               |                                     |
| Yes       | 150014 | Hydrazine sulfate  | DNA methylation   | Alkyl        | PMID: 8048059                 |                                     |
| Yes       | 102627 | Yoshi-864  | Alkylating Agent  | Alkyl        | PMID: 206359                  |                                     |
| Yes       | 178248 | Chlorozotocin  | Chloroethylating agent  | Alkyl        | PMID: 3335046                 |                                     |
| Yes       | 73754  | Fluorodopan  | Alkylating Agent  | Alkyl        |                               |                                     |
| Yes       | 95441  | Methyl CCNU  | Alkylating Agent  | Alkyl        | PMID: 2818619                 |                                     |
| Yes       | 296934 | Teroxirone   | Alkylating Agent  | Alkyl        | PMID: 6478450                 |                                     |
| Yes       | 241240 | Carboplatin  | Platinum-DNA adduct   | Alkyl        | PMID: 10626357                |                                     |
|           | 104800 | Dibromodulcitol  | An alkylating antitumor drug  | Alkyl        | PMID: 3699079                 |                                     |
| Yes       | 172112 | Spiromustine(spirohydantoin mustard)   | Alkylating, lipophilic  | Alkyl        | PMID: 6381379                 |                                     |
| Yes       | 167780 | Asaley   | Alkylating Agent  | Alkyl        |                               |                                     |
| Yes       | 329680 | Hepsulfam  | Alkylates DNA and forms interstrand cross-links.  | Alkyl        | PMID: 9895121 ; PMID: 7882358 |                                     |
| Yes       | 344007 | a piperazine   | Alkylating Agent  | Alkyl        |                               |                                     |
| Yes       | 132313 | Dianhydrogalactitol  | Alkylating Agent  | Alkyl        | PMID: 3699079                 |                                     |
| Yes       | 77213  | Procarbazine   | Methylating agent   | Alkyl        | PMID: 9516945                 |                                     |
| Yes       | 182986 | AZQ  | Alkylating Agent  | Alkyl        | PMID: 9790684                 |                                     |
| Yes       | 602668 | Carmethizole   | Alkylates exclusively at guanine residues via the 2-amino group   | Alkyl        | PMID: 9822545                 | Yes                                 |
| Yes       | 109724 | Iphosphamide   | Prodrug that undergoes extensive P450-catalyzed metabolism  | Alkyl        | PMID: 10692561                |                                     |

|     |         |  |   |                                  |                                 |     |
|-----|---------|--|---|----------------------------------|---------------------------------|-----|
| Yes | 338947  | Clomesone  | Chloroethylating agent  | Alkyl                            | PMID: 8382507                   |     |
| Yes | 353451  | Mitozolamide (Azolastone)  | Alkylating agent, O6-methylguanine-DNA methyltransferase deficient cells are more sensitive   | Alkyl                            | PMID: 3470008                   |     |
| Yes | 2711674 | Carboxyphthalato platinum  | Platinum alkylating agent   | Alkyl                            |                                 |     |
| Yes | 363812  | Tetraplatin  | Platinum alkylating agent   | Alkyl                            | PMID: 9566723                   |     |
| Yes | 3088    | Chlorambucil   | Alkylating Agent  | Alkyl                            | PMID: 7862715                   |     |
| Yes | 361456  | Pyrazine diazohydroxide  | Forms DNA adducts via the reactive pyrazine diazonium ion   | Alkyl                            | PMID: 9563886                   |     |
|     | 362856  | Temozolomide   | Methylating agent, produces O(6)-methylguanine DNA adducts  | Alkyl                            | PMID: 11489806                  |     |
| Yes | 25154   | Pipobroman   | Alkylating Agent  | Alkyl                            | Micromedex                      |     |
| Yes | 256927  | CHIP   | Platinum alkylating agent   | Alkyl                            | PMID: 7193043                   |     |
| Yes | 9706    | Triethylenemelamine  | Alkylating Agent  | Alkyl                            | PMID: 8781576                   |     |
|     | 14210   | Melphalan  | Alkylating agent Bulky adduct, subject to NER   | Alkyl                            | PMID: 9893669                   |     |
| Yes | 135758  | Piperazinedione  | Alkylating Agent  | Alkyl                            | PMID: 348078                    |     |
| Yes | 6396    | Thio-tepa  | Alkylating Agent  | Alkyl                            | PMID: 10493531                  |     |
| Yes | 349438  | 4-Ipomeanol  | Activated by cytochrome P450 monooxygenases into highly toxic alkylating metabolites  | Alkyl                            | PMID: 9650611                   |     |
| Yes | 750     | Busulfan   | Alkylating Agent  | Alkyl                            | PMID: 9780133                   |     |
| Yes | 348948  | Cyclodisone  | Alkylating Agent  | Alkyl                            | PMID: 2908842                   |     |
| Yes | 34462   | Uracil nitrogen mustard  | Alkylating Agent  | Alkyl                            | PMID: 1620613                   |     |
|     | 683863  | MGI 114 (6-hydroxymethylacylfulvene, HMAF)   | Alkylation of DNA, increased cytotoxicity in DNA repair-deficient cell lines, and potent inhibition of DNA synthesis. Additional studies have shown that MGI 114 produces cell-cycle arrest at the S-phase, initiation of single-stranded DNA breaks          | Alkyl                            | PMID: 11023607                  | Yes |
|     | 697726  | RH1  | RH1 is efficiently bioactivated by DT-diaphorase. It is selectively cytotoxic to cells with high DT-diaphorase activity, and nontoxic toward cells with low levels of the enzyme. The mechanism of action involves the production of hydroquinone             | Alkyl                            | PMID: 9865924                   | Yes |
| Yes | 142982  | Hycanthone methane sulfate   | analog of nsc134434: Alkylating ( intercalating)  | Alkyl                            |                                 |     |
| Yes | 762     | Nitrogen mustard   | The bifunctional alkylating anticancer drug nitrogen mustard forms a variety of DNA lesions, including monoadducts and intrastrand and interstrand crosslinks.  | Alkyl                            | PMID: 10454632                  |     |
|     | 106408  | Anthramycin methyl ether   | DNA minor groove binder, alkylates guanine at N-2.  | Alkyl                            | PMID: 8873596                   | Yes |
|     | 134679  | RH1 analog   |   | Alkyl                            |                                 | Yes |
|     | 360702  | RH1 analog   |   | Alkyl                            |                                 | Yes |
| Yes | 56410   | Porfiromycin   | Alkylating, mitomycin derivative  | Alkyl                            | PMID: 8552660                   | Yes |
|     | 684681  | EF5  | A fluorinated 2-nitroimidazole. EF5 undergoes reductive metabolism in hypoxic cells, leading to reactive nitroso and hydroxylamine species which bind to cellular protein thiols. The extent of binding or adduct formation is inversely proportional to cell | Alkyl                            | PMID: 10766193                  | Yes |
|     | 1026    | Cycloleucine   | Inhibitor of methionine adenosyltransferase   | Amino acid                       | PMID: 7953605                   |     |
| Yes | 83265   | Tritly cysteine  | Potential inhibitory activity on aminoacyl-tRNA synthetases   | Amino acid                       | PMID: 2619514                   |     |
| Yes | 303861  | L-cysteine analog  | L-cysteine analog   | Amino acid                       |                                 |     |
| Yes | 224131  | N-(phosphonoacetyl)-L-aspartate (PALA)   | Amino acid analog   | Amino acid                       |                                 |     |
| Yes | 7365    | L-Norleucine   | An unnatural amino acid   | Amino acid                       |                                 |     |
|     | 6224    | p-Bromophenacyl bromide  | A histidine modifying reagent   | Amino acid                       | PMID: 10348910                  |     |
|     | 116328  | Furanomycin  | Nonprotein amino acid, an isoleucine antagonist   | Amino acid                       | PMID: 2182633                   |     |
| Yes | 347512  | Flavone acetic acid  | Inhibits proliferation of endothelial cells by a superoxide-dependent mechanism and induces apoptosis by a nitric oxide and superoxide-independent mechanism.   | Angiogenesis                     | PMID: 10953282                  |     |
|     | 66847   | Thalidomide  | Thalidomide has been shown to possess anti-inflammatory as well as antiangiogenic and differentiation-inducing properties.  | Angiogenesis                     | PMID: 11448901                  | Yes |
|     | 626201  | PENTOSAN SULFATE   | A sulfated polysaccharide that inhibits the in vitro growth, proliferation, and migration of endothelial cells induced by fibroblast growth factor  | Angiogenesis                     | PMID: 11217082 ; PMID: 10402490 | Yes |
|     | 639366  | 1-[[3-(diethylamino)-2-hydroxypropyl]amino]-4-[(2,3- epoxypropyl)amino]-9,10-anthracenedione fumaric acid salt | A diaminoantraquinone inhibitor of angiogenesis; reversibly inhibits bovine endothelial cell growth with an IC50 that ranged between 1 and 4 nM   | Angiogenesis                     | PMID: 7525934                   | Yes |
|     | 141538  | Ovalicin   | Angiogenesis inhibitor  | Angiogenesis                     | PMID: 9860943                   | Yes |
|     | 659853  | 2-Methoxyestradiol   | It inhibits tubulin depolymerization by binding to microtubules at the colchicine binding site. directly inhibits both basic fibroblast growth factor (bFGF)- and vascular endothelial cell growth factor (VEGF)-induced angiogenesis.                        | Angiogenesis; Estradiol; Tubulin | PMID: 11505393                  | Yes |
| Yes | 139105  | Triazine   | Antifolate  | Antifol                          | PMID: 3431593                   |     |

|          |        |  |  |                     |  |     |
|----------|--------|--|--|---------------------|--|-----|
| Yes      | 139490 | DL-N5-Methyltetrahydrohomofolate   | A folate antagonist of relatively low toxicity   | Antifol             | PMID: 6848202                            |     |
| Yes      | 127755 | Triazine related   | Antifolate   | Antifol             | PMID: 3431593                            |     |
| Yes      | 740    | Methotrexate   | Antifolate, inhibits dihydrofolate reductase   | Antifol             | PMID: 9281432                            |     |
|          | 19494  | Metoprine  | Lipid soluble DHFR inhibitor   | Antifol             | PMID: 7592937                            |     |
| Yes      | 352122 | Trimetrexate   | Lipophilic antifolate  | Antifol             | PMID: 10091649                           |     |
| Yes      | 95678  | 3-HP   | DNA Antimetabolite   | Antimetab           |  |     |
| Yes      | 126771 | Dichlorallyl lawsone   | Inhibits dihydroorotate dehydrogenase  | Antimetab           | PMID: 10658902                           |     |
| Yes      | 107392 | 5-HP   | DNA Antimetabolite   | Antimetab           |  |     |
|          | 159548 | Mimosine   | A prolyl 4-hydroxylase inhibitor; a DNA synthesis initiator poison; inhibits both initiation and elongation of DNA synthesis; through iron chelation blocks cell cycle progression   | Antimetab           | PMID: 9056424                            |     |
|          | 234714 | Aphidocolin  | DNA replication inhibitor  | Antimetab           | PMID: 10655588                           |     |
| Yes      | 312887 | Fludarabine phosphate  | A DNA synthesis inhibitor with potent immunosuppressive activity and minimal clinical toxicity; primer RNA chain termination is the major effect responsible for the inhibition of RNA-primed DNA synthesis; DNA polymerase delta is able to excise the incorp | Antimetab           | PMID: 1699280                            |     |
| Yes      | 368390 | Brequinar (DUP785)   | Dihydroorotate inhibitor   | Antimetab           | PMID: 11329288                           |     |
|          | 169627 | Streptovar C   | Inhibition of terminal deoxynucleotidyltransferase activity  | Antimetab           | PMID: 26862                              |     |
| Yes      | 303812 | Aphidicolin glycinate  | An inhibitor of DNA polymerases alpha and delta  | Antimetab           | PMID: 8306334                            |     |
| Yes      | 23759  | Delta-1-testololactone   | Aromatase inhibitor  | Aromatase           | PMID: 7949205                            |     |
|          | 170986 | Miconazole   | Aromatase inhibitor  | Aromatase           | PMID: 9502046                            |     |
|          | 2770   | Oxamide  | Calcium oxalate binding protein inhibitor  | Ca++                | PMID: 9453008                            |     |
|          | 11926  | Aristolochic acid  | An inhibitor of Ca2+-ionophore-stimulated phospholipase A2   | Ca++                | PMID: 10444641                           |     |
|          | 62323  | 1-Piperazineethanol, 4-[3-[2-(trifluoromethyl)phenothiazin-10-yl]propyl]-, dihydrochloride | Calmodulin antagonist  | Ca++                | PMID: 11223176                           |     |
| Yes      | 77037  | Tetrandrine  | Tetrandrine is a wide-spectrum calcium channel antagonist.   | Ca++ channel        | PMID: 9606031                            |     |
|          | 351907 | Mastoparan   | Amphiphilic peptide, a potent inhibitor of the sarcoplasmic reticulum Ca2+-ATPase.   | Ca++ channel        | PMID: 10329678                           | Yes |
| discreet |        |  | Blocks Ca(2+)-activated K(+) channels  | Ca++ channel        |  | Yes |
|          | 17474  | Trifluoperazine dihydrochloride  | Calmodulin antagonist; DNA protein kinase inhibitor  | Ca++; Kinase        | PMID: 10625668 ; AACR 2001 absstact 1097 |     |
|          | 705701 | 9 NITROPAULLONE  | A potent inhibitor of cyclin-dependent kinases (CDKs), specifically CDK1, CDK2, and CDK5.  | CDK                 | PMID: 10888036                           | Yes |
|          | 608776 |  | Rohitukine analogs: Flavopiridol is a novel semisynthetic flavone derivative of the alkaloid rohitukine. Flavopiridol is known to inhibit potently the activity of multiple cyclin-dependent kinases.  | CDK                 | PMID: 9516149                            | Yes |
|          | 29606  |  | A CDK inhibitor  | CDK                 | Supplier                                 |     |
|          | 649890 | Flavopiridol   | Inhibits most cyclin-dependent kinases (cdks); inactivates transcription elongation factor p-tefb  | CDK                 | PMID: 11431468                           | Yes |
|          | 29603  |  | A CDK inhibitor  | CDK                 | Supplier                                 |     |
|          | 51350  |  | Rohitukine analog: Flavopiridol is a novel semisynthetic flavone derivative of the alkaloid rohitukine. Flavopiridol is known to inhibit potently the activity of multiple cyclin-dependent kinases.   | CDK                 | Supplier                                 | Yes |
|          | 46387  |  | A CDK inhibitor  | CDK                 | Supplier                                 | Yes |
|          | 51023  |  | CDK active   | CDK                 | Supplier                                 | Yes |
|          | 29605  |  | A CDK inhibitor  | CDK                 | Supplier                                 | Yes |
|          | 5036   | Caffeine   | Caffeine inhibits the checkpoint kinase ATM and ATR kinase   | Checkpoint ; Kinase | PMID: 10485486                           |     |
|          | 666076 | Piroxicam  | selective COX1 inhibitor   | Cyclooxygenase      | PMID: 10970676                           | Yes |
|          | 4060   | Ursolic acid   | Selective inhibitor of cyclooxygenase-2; Inhibits HIV-1 protease; Inhibits chitin synthase II from <i>S. cerevisiae</i>  | Cyclooxygenase      | PMID: 9784154                            | Yes |
| Yes      | 13875  | Hexamethylmelamine   | A crosslinking agent   | DNA binding         | PMID: 7586186                            |     |
| Yes      | 322921 | Pibenzimol HCl   | DNA minor groove binder  | DNA binding         | PMID: 7539521                            |     |
| Yes      | 305884 | Acodazole  | Intercalater   | DNA binding         | PMID: 2429695                            |     |
|          | 143020 | Mithramycin magnesium salt   | Transcription inhibitor, which binds reversibly to DNA in the presence of divalent metal ions such as Mg2+.  | DNA binding         | PMID: 10102989                           |     |
|          | 640506 | BE-4-4-4-4   | Depletes cellular polyamines and alters chromatin structure  | DNA binding         | PMID: 10071986                           | Yes |
|          | 38270  | Olivomycin   | GC-specific DNA binding fluorochrome   | DNA binding         | PMID: 7518377                            |     |

|          |                 |  |   |                         |                |     |
|----------|-----------------|--|---|-------------------------|----------------|-----|
|          | 194350          | Acridine Orange  | DNA-intercalating fluorophore   | DNA binding             | PMID: 10425339 |     |
|          | 289487          | Asterriquinone   | Interstrand cross-links intercalates, causes G1 arrest  | DNA binding             | PMID: 9413222  |     |
|          | 71047           | Trioxsalen   | DNA crosslink   | DNA binding             | PMID: 9134753  | Yes |
| Yes      | 526417          | Echinomycin  | DNA binding, bis-intercalating antibiotic   | DNA binding             | PMID: 7688090  | Yes |
| Yes      | 58514           | Chromomycin A3   | Chromomycin A3 is a G/C-rich minor groove DNA binding agent that blocks macromolecular synthesis via reversible interaction with DNA.   | DNA binding             | PMID: 9827579  | Yes |
|          | 37132           | Chrysophanic acid  | Inhibitor of cAMP-dependent protein kinase; Intercalater  | DNA binding ; Kinase    | PMID: 7582818  |     |
| Yes      | 3053            | Actinomycin D  | DNA binding; inhibits Shc/Grb2 interaction  | DNA binding ; Other     | PMID: 10403397 |     |
|          | 125066          | Bleomycin  | Besides cleaving DNA, in vitro, Fe-bleomycin cleaves the anticodon of yeast tRNA(Phe) specifically  | DNA breaks              | PMID: 7682070  |     |
|          | 159633          | Neocarzinostatin   | Nucleic acid bulges have been implicated in a number of biological processes and are specific cleavage targets for the enediyne antitumor antibiotic neocarzinostatin   | DNA breaks              | PMID: 10194353 |     |
|          | 295565          | Kidamycin  | DNA binding; single-strand scission of DNA  | DNA breaks              | PMID: 942683   | Yes |
| Yes      | 104801          | Cytembena  | Dose-dependent DNA repair responses   | DNA damage              | PMID: 2169015  |     |
| Yes      | 119875          | Cis-platinum   | DNA cross-linking agent   | DNA damage              | PMID: 9371511  |     |
| Yes      | 338720          | Penclomedine   | May be metabolized to a free radical, DNA-reactive species.   | DNA damage              | PMID: 7488229  |     |
| Yes      | 26271           | Cyclophosphamide   | DNA damage by DNA cross-linking   | DNA damage              | PMID: 9042403  |     |
| Yes      | 164011          | Rubidazone   | Interstrand DNA crosslinks  | DNA damage              | PMID: 8031321  |     |
|          | 400978          | Illudin M  | Activity against even multi-drug resistant; DNA damage, ERCC2 and ERCC3 helicases are critical for repair; inhibition of DNA synthesis  | DNA damage              | PMID: 8053936  |     |
|          | 9221            | Quercitrin   | Competitive inhibitor of DNA-dependent protein kinase, role in DNA repair   | DNA damage ; Kinase     | PMID: 10363977 | Yes |
|          | 683551          | COL-3 (6-demethyl-6-deoxy-4-dedimethylaminotetracycline) | COL-3 is a matrix metalloproteinase (MMP) inhibitor.  | ECM ; Metalloproteinase | PMID: 11208854 | Yes |
|          | 49083           | Sitosterol   | A phytoestrogen   | Estrogen                | PMID: 10069478 |     |
| Yes      | 321803          | 4-Nitroestrone 3-methyl ether                            | Binds estrogen receptor   | Estrogen                |                |     |
| Yes      | 180973          | Tamoxifen  | Non-steroidal antiestrogen  | Estrogen                | PMID: 10411386 |     |
|          | 3070            | Diethylstilbestrol                                       | Synthetic estrogen, induces multipolar spindles   | Estrogen ; Spindle      | PMID: 10656490 |     |
|          | 261037          | Misonidazole   | Sensitizes hypoxic cells to radiation by a free radical mechanism   | Free radical            | PMID: 10506720 |     |
|          | 6152            | Chrysarobin  | Tumor promoter, may act through a free radical mechanism.   | Free radical            | PMID: 8640943  |     |
|          | 85236           | Heleinalin   | Potent hydroxyl radical scavenger, selectively alkylates the p65 subunit of NF-kappaB   | Free radical            | PMID: 10364836 |     |
|          | 9220            | Rutin  | Bioflavonoid, free radical scavenger  | Free radical            | PMID: 10578483 | Yes |
|          | 400639          | Glutathione  | Glutathione   | Glutathione             |                |     |
| Yes      | 326231          | L-buthionine sulfoximine                                 | A specific inhibitor of glutathione biosynthesis ( a specific inhibitor of gamma-glutamylcysteine synthetase)   | Glutathione             | PMID: 10515588 |     |
|          | 92859           | Arsenic Trioxide   | The Cpp32-dependent apoptotic pathway induced by AsTO appears to be regulated by three enzymes: glutathione peroxidase (GPx), which reduces H2O2; glutathione S-transferase (GST), which can transport AsTO out of the cell; and intracellular catalase, whic | Glutathione             | PMID: 10428472 | Yes |
|          | 1214            | Triphenyl tin  | Glutathione-S-transferase inhibitor   | Glutathione             | PMID: 3468922  | Yes |
|          | 614552          | CASTANOSPERMINE  | An inhibitor of glucosidases I and II   | Glycosylation           | PMID: 10984471 | Yes |
|          | 177382          | Tunicamycin  | Blocks the first step in the biosynthesis of N-linked oligosaccharides  | Glycosylation           | PMID: 10531415 |     |
|          | 267431          | Amphotomycin   | Blocks the formation of GlcNAc-lipids   | Glycosylation           | PMID: 9613828  |     |
|          | 706995          | MS-27-275  | A histone deacetylase (HDA) inhibitor   | Histone deacetyl        | PMID: 10200307 | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Inhibits histone deacetylase activity   | Histone deacetyl        | PMID: 11126357 | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| 174280   | Sodium butyrate | Histone deacetylase inhibitor                            | Histone deacetyl  | PMID: 10200307          |                |     |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| discreet |                 |  | Shown to inhibit histone deacetylase activity   | Histone deacetyl        | Supplier       | Yes |
| Yes      | 356894          | Deoxyspergualin  | Blocks nuclear translocation of NF-KB; binds HSP70 and HSP90  | Hsp90                   | PMID: 11278929 |     |
|          | 122750          | Geldanamycin   | Binds to the Hsp90 chaperone protein  | Hsp90                   | PMID: 9817749  | Yes |
|          | 330507          | 17AAG  |   | Hsp90                   |                | Yes |

|     |          |   |   |                                  |                           |     |
|-----|----------|---|---|----------------------------------|---------------------------|-----|
|     | 74489    |   | Integrase inhibitor   | Integrase                        | Supplier                  |     |
|     | 122023   | Valinomycin                             | A K+ ionophore  | Ion channel                      | PMID: 10564350            |     |
|     | 36724    | Tetraethylammonium                      | Inhibitor of voltage-dependent K+ channels  | Ion channel                      | PMID: 11219402            |     |
|     | 85791    | Ethacrynic acid                         | A potassium ion channel blocker   | Ion channel                      | PMID: 10325579            |     |
|     | 25485    | Ouabain                                 | Sodium pump inhibitor   | Ion channel                      | PMID: 10605438            |     |
|     | 71935    | Duramycin                               | Forms ion channels in both artificial and biological membranes. Inhibit phospholipase A2 indirectly by specifically sequestering the substrate phosphatidylethanolamine.  | Ion channel                      | PMID: 1377492             |     |
| Yes | 325319   | Didemnin B                              | Inhibits palmitoyl protein thioesterase. Dynamic protein palmitoylation has been proposed to regulate GTP-binding proteins binding proteins by controlling their membrane association and thus their access to key signaling proteins | Isoprenyl                        | PMID: 9671519             |     |
|     | 706470   |   | Farnesyl transferase inhibitor  | Isoprenyl                        | Supplier                  | Yes |
|     | 712392   |   | Farnesyltransferase inhibitor   | Isoprenyl                        | AACR 2001 abstract # 2631 | Yes |
|     | 106997   | Lipoxamycin;U 26146D                    | Inhibition of serine palmitoyl-transferase activity   | Isoprenyl                        | PMID: 8175492             | Yes |
|     | discreet |   | Inhibition of farnesyl protein transferase  | Isoprenyl                        |                           | Yes |
|     | 407436   | Chrysin                                 | Inhibits casein kinase II   | Kinase                           | PMID: 9177178             |     |
|     | 17468    | Promazine                               | DNA protein kinase inhibitor  | Kinase                           | AACR 2001 abstact 1097    |     |
|     | 32982    | Curcumin                                | A potent inhibitor of the COP9 signalosome kinase activity (which has homology to regulatory subunits of the proteasome   | Kinase                           | PMID: 10363643            |     |
|     | 221019   | Wortmannin                              | a potent PI 3'-kinase inhibitor; significantly decreased the effect of EGF; noncompetitive inhibitor of DNA-dependent protein kinase involved in DNA repair , with a Ki of 120 nM   | Kinase                           | PMID: 10363977            | Yes |
|     | 654705   |   | bcr/abl kinase inhibitor  | Kinase                           | PMID: 10656455            | Yes |
|     | 680410   | adaphostin                              | bcr/abl kinase inhibitor  | Kinase                           | PMID: 10656455            | Yes |
|     | 638850   | UCN-01 (7hydroxystaurosporine)          | A G2-checkpoint inhibitor; a potent protein kinase inhibitor  | Kinase                           | PMID: 10786669            | Yes |
|     | 56346    | Rottlerin                               | Rottlerin is a Protein Kinase C-delta inhibitor.  | Kinase ; PKC                     | PMID: 8123051             | Yes |
|     | 65689    | Boldine                                 | Neuromuscular blockade; potent inhibitor of calmodulin dependent myosin light chain kinase  | Kinase ; Signalling              | PMID: 9434598             |     |
|     | 93135    | Oxyacanthine                            | Potent lipoxygenase inhibitor   | Lipoxygenase                     | PMID: 8941945             |     |
|     | 26428    | Esculetin                               | Lipoxygenase inhibitor; Esculetin suppresses proteoglycan metabolism by inhibiting the production of matrix metalloproteinases  | Lipoxygenase ; Metalloproteinase | PMID: 10334506            |     |
| Yes | 3051     | N-methylformamide                       | Cytoskeleton-dependent surface blebbing; Modulates the expression of some adhesion receptors, cell adhesion to laminin, collagen I, vitronectin and fibrinogen  | Memb                             | PMID: 1426160             |     |
|     | 71936    | Cinnamycin                              | Inhibit phospholipase A2 indirectly by specifically sequestering the substrate phosphatidylethanolamine.  | Memb                             | PMID: 1741778             |     |
|     | 335308   | Cimetidine                              | An H2 receptor histamine antagonist   | Memb recept                      | PMID: 11219402            |     |
|     | 19509    | Yohimbine                               | Alpha 2-adrenoceptor antagonist   | Memb recept                      | PMID: 9444525             |     |
|     | 407282   | Cytisine                                | Nicotinic AchR agonist  | Memb recept                      | PMID: 9118208             |     |
|     | 32865    | Carbachol                               | Muscarinic acetylcholine receptor (a G-protein-coupled receptor) agonist  | Memb recept                      | PMID: 11222647            |     |
|     | 107413   | Securinine                              | Antagonist of the GABAergic receptor  | Memb recept                      | PMID: 1317920             | Yes |
|     | 170984   | Pimozide                                | Targeted D2 dopamine receptor   | Memb recept                      | PMID: 10548412            | Yes |
|     | 59272    | Reserpine                               | An inhibitor of multidrug efflux pumps  | Memb transport                   | PMID: 10052906            |     |
|     | 2833     | Phloridzin                              | Sugar transport inhibitor   | Memb transport                   | PMID: 10480331            | Yes |
|     | 2039     | 8-hydroxyquinoline                      | Metal chelating agent   | Metal                            | PMID: 8631142             |     |
|     | 176      | DIPICOLINATE                            | A chelator of zinc ion  | Metal                            | PMID: 11156471            |     |
|     | 18805    | Thujaplicin alpha                       | Siderophore, copper chelater  | Metal                            | PMID: 9806486             | Yes |
|     | 4265     | 1, 10-Phenanthroline, monohydrochloride | Metalloproteinase inhibitor   | Metalloproteinase                | PMID: 10556832            |     |
| Yes | 4728     | Aminothiadiazole                        | Stromelysin metalloproteinase inhibitor; ATDA is an inosine-5-monophosphate dehydrogenase inhibitor; thus, it prevents synthesis of guanosine monophosphate.  | Metalloproteinase; Antimetab     | Supplier                  |     |
|     | 65690    | Agaric Acid                             | Blocks mitochondrial inner membrane anion channel   | Mitochondria                     | PMID: 7511601             |     |
|     | 26258    | Rotenone                                | Mitochondrial complex I inhibitor   | Mitochondria                     | PMID: 10597238            |     |
|     | 5889     | I-Usnic acid                            | Usnic acid caused complete uncoupling of mitochondrial oxidative phosphorylation. L-usnic acid inactivates urease. L-usnic acid binds to D-fructose-6-P aminotransferase.   | Mitochondria                     | PMID: 8726330             |     |
|     | 106193   | Fusarubin                               | Oxidizer and inhibitor of mitochondrial NADH:ubiquinone reductase.  | Mitochondria                     | PMID: 1497345             |     |
|     | 58239    | Antimycin A3                            | Inhibition of mitochondrial electron transport  | Mitochondria                     | PMID: 2517475             |     |
|     | 76455    | Peliomycin                              | Inhibitor of the mitochondrial ATPase   | Mitochondria                     | PMID: 6242755             | Yes |

|     |        |   |   |                         |  |     |
|-----|--------|---|---|-------------------------|--|-----|
| Yes | 148958 | Florafur (pro-drug)                                     | Nucleoside fluoro analog  | Nucleoside              |  |     |
| Yes | 71851  | alpha-Thiodeoxyguanosine                                | Guanosine analog  | Nucleoside              |  |     |
| Yes | 126849 | 3-Deazauridine  | CTP synthetase inhibitor  | Nucleoside              | PMID: 7575666  |     |
| Yes | 145668 | Cyclocytidine   | Cyclocytidine is an analog of cytidine and acts as an antimetabolite, interfering with nucleic acid synthesis. In addition, cyclocytidine is an adrenergic agonist.   | Nucleoside              | PMID: 4738486  |     |
| Yes | 21548  | Deoxythymidine  | Nucleoside  | Nucleoside              |  |     |
| Yes | 755    | Thiopurine  | Nucleoside analog. The inherited deficiency of thiopurine methyltransferase (1/300 people) leads to severe myelosuppression in homozygous patients treated with thiopurine derivatives.   | Nucleoside              | PMID: 11067806   |     |
| Yes | 63878  | ara-C   | Cytosine analog   | Nucleoside              |  |     |
| Yes | 37364  | O6-Methylguanine  | O6-Methylguanine  | Nucleoside              |  |     |
| Yes | 286193 | Tiazofurin  | An oncolytic C-nucleoside, inhibits IMP dehydrogenase activity, decreases cellular GTP pools, and downregulates ras gene expression; S phase arrest; lowering of the activity of PLC  | Nucleoside              | PMID: 10413291   |     |
|     | 112907 | THU (tetrahydouridine) -                                | A cytidine deaminase inhibitor  | Nucleoside              | PMID: 9771951  |     |
| Yes | 118994 | Inosine glycodialdehyde                                 | analog of nsc20262: Inosine; Nucleoside   | Nucleoside              |  |     |
| Yes | 281272 | Ara AC  | Nucleoside  | Nucleoside              |  |     |
|     | 98700  | Adenosine, 2' 3'-dideoxy                                | P-site inhibition of adenylyl cyclase   | Nucleoside              | PMID: 11087399   |     |
|     | 143647 | Alanosine DL  | An inhibitor of de novo AMP synthesis   | Nucleoside              | PMID: 10197619   |     |
| Yes | 261726 | 3-Deazaguanine  | 3-Deazaguanine  | Nucleoside              |  |     |
| Yes | 19893  | 5-fluorouracil  | An inhibitor of pyrimidine synthesis which specifically depletes dTTP pools   | Nucleoside              |  |     |
|     | 749    | 8-Azaguanine  | Synthetic analog of guanine, lethal to cells with normal hypoxanthine phosphoribosyltransferase (HPRT) activity   | Nucleoside              | PMID: 7273856  |     |
| Yes | 102816 | 5-azacytidine   | RNA/DNA Antimetabolite  | Nucleoside              |  | Yes |
| Yes | 264880 | 5,6-dihydro-5-azacytidine                               | RNA/DNA Antimetabolite  | Nucleoside              |  |     |
| Yes | 752    | Thioguanine   | Guanine analog. The delayed cytotoxicity of thioguanine involves the postreplicative DNA mismatch repair system. Mismatch repair deficient cells are resistant. MutS binds to DNA containing thioguanine. Bioactivated by hypoxanthine-guanine phosphoribosyl | Nucleoside              | PMID: 8688098<br>PMID: 9855005<br>PMID: 9054555<br>PMID: 9262380 |     |
| Yes | 280594 | Triciribine phosphate                                   | Inhibited de novo purine nucleotide synthesis, GTP more than ATP; even though triciribine is a nucleoside chemically, it does not act biologically by classic nucleoside modalities   | Nucleoside              | PMID: 2480792  |     |
|     | 65423  | Nebularin   | Nebularin is an analogue of adenosine and a competitive inhibitor of adenosine deaminase.   | Nucleoside              | PMID: 3607008  |     |
| Yes | 291643 | Pyrimidine-5-glycodialdehyde                            | Nucleoside  | Nucleoside              |  |     |
| Yes | 71261  | Thioguanine deoxyriboside                               | Guanine analog  | Nucleoside              |  |     |
|     | 118090 | Isoxanthopterin   | Highly fluorescent guanosine analog   | Nucleoside              | PMID: 7659509  |     |
| Yes | 375575 | Cyclopentenylcytosin                                    | A pyrimidine poison   | Nucleoside              |  | Yes |
| Yes | 153353 | L-alanosine   | An inhibitor of de novo AMP synthesis   | Nucleoside              | PMID: 10197619   |     |
|     | 167897 | Adenosine, 3-deaza-                                     | analog of nsc7652: Nucleoside   | Nucleoside              |  |     |
|     | 94017  | cAMP  | analog of nsc7652: Nucleoside   | Nucleoside              |  |     |
|     | 146604 | Uridine, 5-fluoro-                                      | analog of nsc20256: Nucleoside  | Nucleoside              |  |     |
| Yes | 284751 | Adenosine, 8-chloro-, cyclic 3',5'-(hydrogen phosphate) | analog of nsc7652: Nucleoside   | Nucleoside              |  |     |
|     | 137442 | Cryptosporiopsin  | Affects uptake and phosphorylation of nucleosides   | Nucleoside              | PMID: 1168526  | Yes |
|     | 316458 | Neplanocin A  | Adenosine analog; A potent inhibitor of S-adenosylhomocysteine hydrolase; leads to inhibition of the in vivo guanine-7-methylation of mRNA cap structure  | Nucleoside ; Prot synth | PMID: 8422953  |     |
| Yes | 32946  | MITOGUAZONE   | Interferes with polyamine synthesis   | Other                   | PMID: 10706462   |     |
| Yes | 95580  | Hexamethylenebisacetamide                               | A potent inducer of differentiation.  | Other                   | PMID: 9458105  |     |
|     | 21206  | 6-Aminonicotinamide                                     | A potent niacin antagonist that is anabolized to 6-amino-nicotinamide-adenine dinucleotide (6-amino-NAD) and has been shown to modulate NAD-dependent repair pathways.  | Other                   | Supplier   |     |
|     | 667219 | Sulfasalazine   | Sulfasalazine is a potent and specific inhibitor of NF-kappaB activation  | Other                   | PMID: 9486988  | Yes |
|     | 179834 | Withanolide E   | analog of Withanolide A: a vimentin intermediate filament-targeting drug  | Other                   | PMID: 7721954  |     |
|     | 18804  | 4-Isopropyltropolone                                    | Inhibition of tyrosine hydroxylase, the first step in dopamine biosynthesis   | Other                   | PMID: 6039447  |     |
| Yes | 163501 | Acivicin  | Gamma glutamyl transpeptidase inhibitor   | Other                   | PMID: 10652029   |     |

|     |        |                                  |   |                        |                |     |
|-----|--------|----------------------------------|---|------------------------|----------------|-----|
| Yes | 314055 | A Nitroimidazole                 | reactive oxygen?  | Oxid                   |                |     |
|     | 7627   | P-aminobenzoic acid              | Photochemical formation of singlet molecular oxygen (oxidative damage)  | Oxid                   | PMID: 8728505  |     |
| Yes | 68075  | Thalcarpine                      | Thalcarpine circumvents multidrug resistance by direct binding to P-glycoprotein.   | Pgp                    | PMID: 8098661  |     |
|     | 79535  | Vanadic acid (HVO3), sodium salt | analog of : P-ATPase inhibitor; transition-state analog of Pgp; phosphotyrosine phosphatase inhibitor   | Pgp , Tyr phosphatase  | PMID: 10672006 |     |
| Yes | 339638 | Fostriecin                       | Inhibits topo II and protein phosphatases involved in cell cycle control. This leads to abnormal centrosomes and abnormal spindles.   | Phosphatase ; Topo II  | PMID: 11376007 |     |
|     | 103645 | Bostrycidin                      | Inhibitor of the Ca(2+)- and calmodulin-dependent cyclic adenosine 3',5'-monophosphate phosphodiesterase  | Phosphodiesterase      | PMID: 1653425  |     |
|     | 36398  | Dihydro-quercetin;Taxifolin      | Stimulates phosphodiesterase with cyclic AMP as the substrate   | Phosphodiesterase      | PMID: 1384499  | Yes |
|     | 95090  | Ergotamine                       | Inhibited the activation of calmodulin-stimulated phosphodiesterase   | Phosphodiesterase      | PMID: 6146911  | Yes |
|     | 31760  | Asperuloside                     | Inhibitor of phosphatidylinositol-3-kinase (2.0 microM)   | PI3K                   | PMID: 7872663  | Yes |
|     | 36405  | Chelerythrine                    | Selective PKC inhibitor   | PKC                    | PMID: 11158244 |     |
|     | 166454 | Dequalinium                      | A PKC inhibitor whose target site was mapped to the catalytic domain.   | PKC                    | PMID: 9756620  |     |
|     | 8661   | Brasilin                         | Inhibits phospholipase A2, protein kinase C, increased glucose transport  | PKC                    | PMID: 9875421  | Yes |
|     | 34266  | Juglone                          | Inhibits protein kinase C; Inactivates the parvulin family of peptidyl-prolyl cis/trans isomerasers   | PKC; Enzymes           | PMID: 9558330  | Yes |
| Yes | 141537 | Anguidine                        | Potent inhibitor of protein synthesis   | Prot synth             | PMID: 999905   |     |
| Yes | 165563 | Bruceantin                       | Protein synthesis inhibitor, binds ribosome   | Prot synth             | PMID: 7707371  |     |
|     | 87432  | Virginiamycin M1                 | Protein synthesis inhibitor; binds specifically to the 50 S ribosomal subunit near the peptidyl transferase center  | Prot synth             | PMID: 7707371  |     |
|     | 4722   | Aloin                            | Inhibits the translation elongation factor eEF-2  | Prot synth             | PMID: 9415207  |     |
| Yes | 141633 | Homoharringtonine                | Protein synthesis inhibitor   | Prot synth             | PMID: 8745664  | Yes |
|     | 337588 | Hikizimycin                      | Inhibits protein synthesis on both pro- and eukaryotic ribosomes by preventing the peptide bond-forming reaction.   | Prot synth             | PMID: 371683   |     |
|     | 3055   | Puromycin Dihydrochloride        | Puromycin, an analog of the 3' end of aminoacyl-tRNA, causes premature termination of translation by being linked non-specifically to growing polypeptide chains.   | Prot synth             | PMID: 10666460 |     |
|     | 292920 | Edeine Sulphate                  | Protein synthesis initiation inhibitor; blocks a specific site on the 40 S ribosomal subunit to which a segment of the methionyl-tRNAsf molecule is bound   | Prot synth             | PMID: 7883007  | Yes |
|     | 18268  | Cactinomycin                     | Protein synthesis inhibitor; Inhibitor of DNA unwinding activity of human DNA helicase II (Ku)  | Prot synth             | PMID: 9535757  | Yes |
|     | 106995 | Lomofungin                       | Inhibits RNA synthesis, both chain initiation and elongation (all 3 polymerases); inhibits polymerase activity solely by chelating the dissociable cations Mn2+ and Mg2+; protein synthesis inhibitor   | Prot synth ; RNA polym | PMID: 1101954  | Yes |
|     | 651714 | KNI 272                          | HIV protease inhibitor  | Protease               | PMID: 11170058 | Yes |
| Yes | 343513 | Dihydro-lenperone                | Protease Inhibitor  | Protease               | Supplier       |     |
|     | 265489 | Bestatin                         | An inhibitor of aminopeptidase N  | Protease               | PMID: 10615014 |     |
| Yes | 237020 | Largomycin                       | Specific proteolytic activity; an acidic protein (pI 4.13, molecular weight 29300)  | Protease               | PMID: 3896321  |     |
|     | 170105 | Macromomycin                     | Protein with aminopeptidase activity  | Protease               | PMID: 3900063  |     |
|     | 118343 | Radicinin                        | Human rhinovirus 3C-protease inhibitor  | Protease               | PMID: 7765405  |     |
|     | 681228 | PS-341 analog                    | Peptidic boronic acid reversibly inhibits the proteasome complex.   | Proteasome             | PMID: 10499643 | Yes |
|     | 681229 | PS-341 analog                    | Peptidic boronic acid reversibly inhibits the proteasome complex.   | Proteasome             | PMID: 10499643 | Yes |
|     | 681239 | PS-341                           | Peptidic boronic acid reversibly inhibits the proteasome complex.   | Proteasome             | PMID: 10499643 | Yes |
|     | 61805  | Cantharidin                      | Inhibitor of serine/threonine protein phosphatases  | Ptase                  | PMID: 10092185 |     |
|     | 34936  | Suramin                          | Suramin is a reversible and competitive protein tyrosine phosphatase inhibitor with Kis values in the low microM range, whereas the Kis for the dual specificity phosphatase VHR is at least 10-fold higher.P2-receptor antagonist; Interacts with G-proteins | Ptase ; Signalling     | PMID: 9575179  |     |
|     | 296961 | Amifostine                       | Chemoprotective aminothiol prodrug, converted to the active compound by membrane-bound alkaline phosphatase.  | Redox                  | PMID: 10360638 |     |
|     | 7887   | Aminoguanidine                   | Inhibits human inducible nitric oxide synthase  | Redox                  | PMID: 10753680 |     |
|     | 87868  | Phenethyl isothiocyanate         | May induce apoptosis through a caspase-3-dependent mechanism; Bcl-2 and Bcl-xL suppressed PEITC-induced apoptosis; an inhibitor of aldehyde dehydrogenases; inhibited cytochrome P450 (P450) isozymes 1A1 and 1A2, 2B1 and 1A2                                | Redox                  | PMID: 9862843  |     |
|     | 59190  | Pinene                           | Monoterpene, inhibition of CYP2B1 monooxygenase   | Redox                  | PMID: 9242356  |     |
|     | 90597  | Diphenyliodonium nitrate         | inhibitor of flavoprotein electron transport  | Redox                  | PMID: 10090757 |     |
|     | 15351  | Vanillin                         | An antigenotoxic agent, sulphotransferase inhibitor   | Redox                  | PMID: 8250957  |     |

|     |        |   |   |                     |                               |     |
|-----|--------|---|---|---------------------|-------------------------------|-----|
| Yes | 133100 | Rifamycin SV  | A potent inducer of cytochrome P-450 oxidative enzymes.   | Redox               | PMID: 9385296                 |     |
|     | 47147  | Prodigiosin   | Prodigiosin facilitates the symport of H+ with Cl- (or exchange of OH- with Cl-) through lysosomal membranes, resulting in uncoupling of vacuolar H+-ATPase.  | Redox               | PMID: 9729483                 |     |
|     | 93131  | Alantolactone   | In vitro inhibitor of the mouse hepatic microsomal mixed-function oxidase   | Redox               | PMID: 2512929                 |     |
|     | 17860  | Dicumarol   | Inhibits DT-diaphorase  | Redox               | PMID: 9324955                 |     |
|     | 38087  | 5-Phenoxy sulphonyl-1-methyl-4-nitroimidazole                                     | A radiosensitizer of hypoxic cells  | Redox               | PMID: 7259957                 | Yes |
|     | 4170   | Vitamin K3  | Inhibits cdc25 phosphatase; Inhibits arginine-specific ADP-ribosyltransferase; a redox cycling compound   | Redox ; Ptase       | PMID: 10207019                |     |
| Yes | 192965 | Spirogermanium  | Organometallic; Addition of 12.5 microM SP to microtubules induced spontaneous disassembly; inhibit the respiratory burst of murine peritoneal macrophages  | Redox ; Tubulin     | PMID: 3829141                 |     |
|     | 11905  | Lapachol  | A vitamin K antagonist, lapachol might target such vitamin K-dependent reactions as the activation of a ligand for the Axl receptor tyrosine kinase; Potent inhibitor of DT-Diaphorase. Inhibition is competitive vs NADH, Ki = 0.15 microM | Redox ; Vit K antag | PMID: 9137445                 |     |
| Yes | 406021 | Ara-6-MP  | Competitive inhibitor of eukaryotic DNA-dependent RNA polymerase II   | RNA polym           | PMID: 6814439                 |     |
| Yes | 15200  | Gallium nitrate   | Inhibits the R2 subunit of ribonucleotide reductase.  | RNR                 | PMID: 9719462                 |     |
| Yes | 1895   | Guanazole   | Guanazole is an inhibitor of ribonucleotide reductase   | RNR                 | PMID: 568630                  |     |
| Yes | 253272 | Caracemide  | Caracemide is an inhibitor of ribonucleotide reductase, and thus an inhibitor of DNA synthesis. Caracemide was found to inhibit choline acetyltransferase.  | RNR                 | PMID: 6395952                 |     |
| Yes | 51143  | Pyrazoloimidazole   | Pyrazoloimidazole is an antimetabolite that specifically inhibits the non-heme iron subunit of ribonucleotide reductase.  | RNR                 | PMID: 1496919                 |     |
| Yes | 32065  | Hydroxyurea   | A ribonucleotide reductase inhibitor  | RNR                 | PMID: 10470093                |     |
|     | 615985 | 2-chloro-5-(2-methyl-5,6-dihydro-1,4-oxathiin-3-yl carboxamido) isopropylbenzoate | A non-nucleoside reverse transcriptase inhibitor  | RT                  | PMID: 9608423                 | Yes |
|     | 641530 | Nevirapine  | Nevirapine is a dipyridodiazepinone and a highly specific inhibitor of HIV-1 RT   | RT                  | PMID: 11486821                | Yes |
|     | 122758 | trans-Retinoic acid   | Retinoic acid   | Signalling          | PMID: 10660575                | Yes |
|     | 4857   | Diethylidithiocarbamate   | Inhibitor of nuclear factor-kappaB  | Signalling          | PMID: 11237996                |     |
|     | 609974 | Carboxyamidotriazole  | A signal transduction inhibitor; an antiangiogenic drug which inhibits both Ca2+ influx and Ca2+ release from intracellular stores  | Signalling          | PMID: 9053505; PMID: 11312104 | Yes |
|     | 91523  | Propranolol   | Phosphatidate phosphohydrolase inhibitor  | Signalling          | PMID: 11230346                |     |
|     | 87221  | Actinomycin C2  | Inhibited Grb2 SH2 domain association   | Signalling          | PMID: 9873474                 |     |
|     | 47151  | Neomycin sulfate  | Phospholipase C inhibitor (10mM)  | Signalling          | PMID: 11232027                |     |
|     | 639966 | Perifosine  | Primarily acts on the cell membrane, where it inhibits signaling through the mitogen-activated protein kinase (MAPK) pathway  | Signalling          | PMID: 10344758                | Yes |
|     | 677411 |   | Inhibits platelet-derived growth factor (PDGF)-mediated signaling   | Signalling          | Supplier                      | Yes |
| Yes | 226080 | Rapamycin   | Selectively binds FKBP12, inhibiting the activity of the TOR/RAFT/FRAP which interferes with the activation of its downstream targets, p70S6 kinase and 4E-BP, resulting in decreased translation of some mRNAs                             | Signalling          | PMID: 11504908                |     |
|     | 34533  | Griseofulvin  | Microtubules were not disassembled by drug treatment, but the spindle organization was disrupted, resulting in tripolar spindles which gave rise to multiple nuclei.  | Spindle             | PMID: 6383831                 |     |
| Yes | 38721  | Mitotane  | A drug that reduces corticosteroid synthesis  | Steroid             | PMID: 11159707                |     |
|     | 10971  | Equilin   | An inhibitor of human type I 17 beta-hydroxysteroid dehydrogenase   | Steroid             | PMID: 10668397                |     |
|     | 5355   | Berberine sulfate   | A moderate inhibitor of telomerase with 50% inhibition at approximately 35 microM.  | Telomerase          | PMID: 10463599                |     |
|     | 364365 |   | Telomerase inhibitor  | Telomerase          | Supplier                      |     |
|     | 48653  |   | Telomerase inhibitor  | Telomerase          | Supplier                      |     |
|     | 363002 |   | Telomerase inhibitor  | Telomerase          | Supplier                      | Yes |
|     | 96349  | Coralyne  | Triplex-stabilizing intercalator; topoisomerase I inhibitor   | Topo I              | PMID: 9485420                 |     |
| Yes | 94600  | Camptothecin  | Stabilizes Topoisomerase I - DNA cleavable complex, leading to DNA breaks   | Topo I              | PMID: 10569939                |     |
| Yes | 609699 | Topotecan   | analog of nsc94600: Camptothecin; Topo I  | Topo I              | PMID: 11497232                | Yes |
| Yes | 100880 | Camptothecin, Na salt   | Stabilizes Topoisomerase I - DNA cleavable complex, leading to DNA breaks   | Topo I              | PMID: 10569939                |     |
|     | 314622 | Topo1A  | Protein-linked DNA strand breaks induced by NSC 314622, a novel noncamptothecin topoisomerase I poison.   | Topo I              | PMID: 9658189                 |     |
|     | 640199 | Rebeccamycin derivative   | analog of nsc359079: Inhibition of topoisomerase I by indolocarbazoles arises in part from their ability to interact with DNA   | Topo I              | PMID: 9092822                 | Yes |

|     |        |                               |   |                                   |                                 |     |
|-----|--------|-------------------------------|---|-----------------------------------|---------------------------------|-----|
| Yes | 208734 | Aclacinomycin A               | DNA binding; Stabilizes Topol-DNA; catalytic inhibitor of Topoll; Proteasome inhibitor  | Topo I ; Topo II-cat ; Proteasome | PMID: 8663210                   |     |
| Yes | 366140 | Pyrazoloacridine              | Inhibits topo I and topo II   | Topo I; Topo II                   | PMID: 9533538                   |     |
|     | 71795  | Ellipticine                   | A topoisomerase II poison - DNA breaks  | Topo II                           | PMID: 7797481                   |     |
| Yes | 320846 | Batracylin                    | Topo II   | Topo II                           | PMID: 7932571                   |     |
| Yes | 249992 | Amsacrine ; m-AMSA            | Topo II poison - DNA breaks   | Topo II                           | PMID: 10497180                  |     |
| Yes | 82151  | Daunorubicin                  | Topoisomerase II poison - DNA breaks  | Topo II                           | PMID: 9763227                   |     |
|     | 279836 | DHAQ ( mitoxantrone)          | Topo II poison  | Topo II                           | PMID: 10497180                  |     |
| Yes | 355644 | Anthrapyrazole                | Topo II Inhibitor   | Topo II                           |                                 |     |
| Yes | 308847 | Amonafide                     | Intercalating agent, Topoisomerase II poison - DNA breaks   | Topo II                           | PMID: 7862525                   |     |
| Yes | 269148 | Menogaril                     | Topo II Inhibitor   | Topo II                           | PMID: 9341219                   |     |
|     | 123127 | Adriamycin; Doxorubicin       | Binds to DNA topoisomerase II, trapping of a covalent enzyme-DNA complex leading to DNA breaks. Mediates free radical damage to DNA and membranes.  | Topo II                           | PMID: 9380029                   |     |
| Yes | 268242 | N,N-dibenzyl daunomycin       | analog of NSC 112758: Topo II Inhibitor   | Topo II                           |                                 |     |
| Yes | 349174 | Oxanthrazole                  | Topo II Inhibitor   | Topo II                           | PMID: 8312123                   |     |
| Yes | 339004 | Chloroquinoxaline sulfonamide | A topoisomerase IIalpha/beta poison   | Topo II                           | PMID: 11085507                  |     |
| Yes | 337766 | Bisantrene HCL                | Topo II Inhibitor   | Topo II                           | PMID: 9855632                   |     |
|     | 311152 | Ellipticine analog            | A water soluble analogue of ellipticine   | Topo II                           | PMID: 2177044                   | Yes |
| Yes | 122819 | VM-26 ; Teniposide            | Topoisomerase II poison - DNA breaks  | Topo II                           | PMID: 9878428                   | Yes |
| Yes | 129943 | ICRF 159                      | Topo II-catalytic inhibitor   | Topo II-cat                       | PMID: 7575679                   |     |
|     | 284356 | Mitindomide                   | Mitindomide is a catalytic/noncleavable complex-forming-type inhibitor of DNA topoisomerase II.   | Topo II-cat                       | PMID: 9351975                   |     |
| Yes | 169780 | ICRF 187                      | Topo II- catalytic inhibitor  | Topo II-cat                       | PMID: 11179439                  |     |
| Yes | 336628 | Merbarone                     | Non-stabilizing Topo II inhibitor, inhibits DNA synthesis, inhibits chromosome separation, causes G2 arrest (but not by DNA breaks)   | Topo II-cat ; Antimetab           | PMID: 10051540                  |     |
|     | 3590   | Calcium leucovorin            | Folate, increases sensitivity to TS inhibitors  | TS                                | PMID: 2500406                   |     |
|     | 24818  | Podophyllotoxin               | Podophyllotoxin binds to tubulin and suppresses microtubule dynamic instability. Podophyllotoxin inhibits nucleoside uptake.  | Tubulin                           | PMID: 7110123                   |     |
| Yes | 757    | Colchicine                    | Binds to tubulin and inhibits microtubule assembly.   | Tubulin                           | PMID: 9578547                   |     |
| Yes | 125973 | Taxol                         | Binds beta-tubulin and promotes microtubule assembly, results in mitotic arrest at the G2/M phase of the cell cycle.  | Tubulin                           | PMID: 9322876                   | Yes |
|     | 613729 | Combretastatin A4             | Tubulin binding   | Tubulin                           | PMID: 11309357                  | Yes |
| Yes | 332598 | Rhizoxin                      | Antimitotic Agent   | Tubulin                           | PMID: 9853684                   |     |
| Yes | 67574  | Vincristine sulfate           | Binds tubulin   | Tubulin                           | PMID: 8639632                   |     |
|     | 330753 | Baccatin III                  | An analogue of Taxol lacking the C-13 side chain, has none of the biological characteristics of Taxol; induced apoptosis independent of cell cycle arrest   | Tubulin                           | PMID: 10747785 ; PMID: 10550564 |     |
|     | 153858 | Maytansine                    | Tubulin binding   | Tubulin                           | PMID: 1287674                   | Yes |
|     | 36586  | Genistein                     | Tyrosine kinase inhibitor   | Tyr kinase                        | PMID: 10656875                  |     |
|     | 610187 | Erbstatin                     | A tyrosine kinase inhibitor   | Tyr kinase                        | PMID: 11223424                  | Yes |
|     | 294734 | Terreic acid                  | A quinone epoxide inhibitor of Bruton's tyrosine kinase   | Tyr kinase                        | PMID: 10051623                  |     |
|     | 93489  | 3-Isothiazolone               | Inhibition of p56(lck) tyrosine kinase by isothiazolones.   | Tyr kinase                        | PMID: 10087161                  | Yes |
|     | 365798 | Piceatannol                   | Tyrosine kinase inhibitor   | Tyr kinase                        | PMID: 11231305                  | Yes |
|     | 696823 |                               | Tyrosine Kinase inhibitor Grb2  | Tyr kinase                        | Supplier                        | Yes |
|     | 696977 |                               | Tyrosine Kinase inhibitor   | Tyr kinase                        | Supplier                        | Yes |
|     | 42470  | PHENYLARSINE OXIDE            | Protein tyrosine phosphatase inhibitor  | Tyr phosphatase                   | PMID: 11278478                  |     |
|     | 89671  | Brefeldin A                   | The fungal toxin brefeldin A dissociates coat proteins from Golgi membranes, causes the rapid disassembly of the Golgi complex and potently stimulates the ADP-ribosylation of the glycolytic enzyme glyceraldehyde-3-phosphate dehydrogenase (GAPDH) | Vescicle                          | PMID: 10331637                  | Yes |
| Yes | 132319 | Indicine N-oxide              |   |                                   |                                 |     |
| Yes | 267213 |                               |   |                                   |                                 |     |
| Yes | 333856 | Antermicin A                  |   |                                   |                                 |     |
| Yes | 293015 |                               |   |                                   |                                 |     |
| Yes | 328426 | Phyllanthoside                |   |                                   |                                 |     |
| Yes | 325014 | Bactobolin                    |   |                                   |                                 |     |
|     | 658586 | cosalane                      | The anti-HIV agent cosalane inhibits both the binding of gp120 to CD4 as well as an undefined postattachment event prior to reverse transcription.  |                                   | PMID: 11262081                  | Yes |

|     |        |                |  |  |  |     |
|-----|--------|----------------|--|--|--|-----|
| Yes | 349156 | Pancratistatin |  |  |  | Yes |
|-----|--------|----------------|--|--|--|-----|